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An effective mean field theory for the coexistence of anti-ferromagnetism and superconductivity: Applications to iron-based superconductors and cold Bose–Fermi atomic mixtures

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ABSTRACT

We study an effective fermion model on a square lattice to investigate the cooperation and competition of superconductivity and anti-ferromagnetism. In addition to particle tunneling and on-site interaction, a bosonic excitation mediated attractive interaction is also included in the model. We assume that the attractive interaction is mediated by spin fluctuations and excitations of Bose–Einstein condensation (BEC) in electronic systems and Bose–Fermi mixtures on optical lattices, respectively. Using an effective mean-field theory to treat both superconductivity and anti-ferromagnetism at equal footing, we study a single effective model relevant for both systems within the Landau energy functional approach and a linearized theory. Within our approaches, we find possible co-existence of superconductivity and anti-ferromagnetism for both electronic and cold-atomic models. Our linearized theory shows while spin fluctuations favor d-wave superconductivity and BEC excitations favor s-wave superconductivity.

1. Introduction

The phenomenon of superconductivity has been an important and rich topic in physics since 1911 when Kamerlingh Onnes discovered that the resistivity of mercury abruptly dropped to zero when it was cooled below 4 K [1]. Over the years, a number of superconducting compounds were found or grown with higher critical temperatures. The highest critical temperature achieved in this class of conventional superconductors was 40 K in magnesium diboride [2]. If one can maintain this resistanceless superconducting state at room temperature, society would obtain huge economic benefits as these compounds can be used to store and transport energy without dissipation. In metal, even though electrons are free to move and provide electrical conduction, energy dissipation occurs due to the resistance coming from electron collisions, lattice vibrations, impurities, and defects. The resistanceless state of these conventional superconductors is explained by the celebrated BCS theory developed by Bardeen, Cooper, and Schrieffer in 1957 [3]. According to the BCS theory, two electrons with equal and opposite speed bind together due to the attractive interaction mediated by the electron–phonon interaction. These bound pairs are called Cooper pairs. As the Cooper pairs are composite bosons, made out of two fermions, Bose–Einstein condensation of these pairs at low temperatures gives resistanceless flow.

The discovery of cuprate superconductors in 1986 by Bednorz and Muller [4] has renovated the interest of superconductivity as these compounds have quite high critical temperatures so they may be useful in practical applications. Immediately after this discovery, several other cuprate superconducting compounds with higher critical temperatures were found [5–8]. Cuprates are considered to be quasi-two dimensional checkerboard lattice materials as the electrons are moving within weakly coupled copper-oxide layers. The highest critical temperature of cuprates at ambient pressure so far is 135 K in mercury barium calcium copper oxide [8]. Then the surprising discovery of iron-based superconductors in 2008 has led to a flurry of activities in the field as these compounds provide more puzzles than answers to the questions of unconventional superconductivity [9]. The critical temperatures of iron-based superconductors are in between that of conventional superconductors and cuprates. The iron based superconductors share some common features with the cuprates. Both are layered materials with 3*d*-electrons. Iron-based superconductors contain layers of iron and pnictogen (arsenic or phosphorus) or chalcogen. Both cuprates and iron based superconductors require chemical or external doping to induce the superconductivity. One of the main differences between these two types of compounds is that the orbital degrees of freedom associate with the Fe-ion in iron-based

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superconductors. Iron based superconductors are essentially multi-orbital systems so that the electron occupation of the d-orbital must be taken into account. In contrast, cuprates can be treated as single orbital systems as the crystal field splitting of d-orbital and valence electronic occupation restrict one hole in the upper most d-orbital.

For both cuprates and iron-pnictides, critical temperatures are too high to be explained by conventional BCS theory. Therefore, the effective interaction for electron pairing must be mediated by excitations rather than conventional phonons. Though it is not completely convincing, there is a general consensus that magnetic or spin fluctuations play the role as the pairing mechanism for these compounds [10]. However, the role of magnetism, the nature of chemical and structural influence, and the pairing symmetry of the electrons are not completely understood. It has been shown that the s-wave pairing is suppressed by ferromagnetic spin fluctuations [11]. However, p-wave pairing can be enhanced by the ferromagnetic spin fluctuations [12]. In both cuprate and pnictide superconductors, the superconductivity always appears in proximity to anti-ferromagnetic (AFM) order or they co-exist in some compounds upon chemical doping. This indicates that the Cooper pairing may be mediated by anti-ferromagnetic fluctuations.

The purpose of this paper is to study the interplay between induced interactions and superconductivity, as well as the competition or cooperation of anti-ferromagnetism and superconductivity. For this purpose, we study both high-temperature superconducting materials and cold atoms in optical lattices. Cold atoms on optical lattices can be considered as quantum simulators for condensed matter electronic systems. One important advantage of using optical lattices to probe fundamental condensed-matter physics problems is that the geometry, dimensionality, and the interaction parameters are under complete control in current experimental setups [13–15]. This high degree of tunability and controllability offers a remarkable opportunity to understand and fully explore the quantum mechanical treatment of cold atomic systems whose behavior is governed by the same underlying many body physics as the materials. In this paper, in addition to the layered high-temperature compounds, we consider a mixture of bosons and two-component fermions in a two-dimensional optical lattice. In experiments, atoms are trapped by combined harmonic trapping and periodic laser potentials. The periodic potentials are created by the interference patterns of intersecting laser beams, and the geometry of the lattice structure can be controlled by the arrangements of the counter propagating lasers. Bose–Fermi mixtures have already been trapped and experimentally studied by several groups [16–27]. A Bose–Fermi mixture, such as a mixture of ^{41}K and two hyperfine states of ^{6}Li or a mixture of ^{6}Li^{40}K bosonic molecule and fermionic species ^{40}K and ^{6}Li is an example of two-component Fermions and single-component bosons system we study here. Such systems have already been experimentally realized in different settings [28–31]. For high-temperature materials, such as cuprates and pnictides, we assume that the effective interaction is caused by spin fluctuations [32,33]. For the Bose–Fermi mixture, we assume that the effective attractive interaction is mediated by the density fluctuations of the bosonic atoms [34–36]. In both cases, the Cooper pairing between Fermi particles can take place due to these boson mediated attractive interactions.

The interplay between superconductivity and anti-ferromagnetism has been investigated in the context of cuprates, organic superconductors, heavy fermion systems [37–42], and iron based superconductors [43–49]. Using a combination of renormalization group and mean-field theory, the competition and coexistence of d-wave superconductivity and antiferromagnetism in the ground state of the two-dimensional Hubbard model has been studied in the context of the cuprates recently [57,58]. The results of this study is in good agreement with the early findings from the dynamical mean field theoretical studies of the ground state of Hubbard model [59–62]. In this work, we develop a simple mean field theory to understand the qualitative physics of the finite temperature coexistence of super conductivity and anti-ferromagnetism relevant for a electronic system and a Bose–Fermi atomic mixture on optical lattices.

The study of anti-ferromagnetism and superconductivity in a lattice model discussed here is somewhat complementary to early studies [38,50,51] and recent studies related to cold atoms [52–56]. However, unlike those studies which assume a generic form of interaction, here we treat explicit momentum dependent interaction relevant for both Bose–Fermi mixtures on optical lattices and related electronic model for iron-based superconductors. Further, we treat both s-wave and d-wave superconducting symmetries at equal footing with their interplay between anti-ferromagnetism. In addition, we point out how one can control the anti-ferromagnetic phase transition to be below or above the superconducting phase transition by controlling the boson density in Bose–Fermi mixtures. In order to study the interplay between superconductivity and anti-ferromagnetism, we develop an effective mean-field theory for an effective fermionic Hamiltonian relevant for both electronic compounds and Bose–Fermi mixtures on two-dimensional lattices. First, we investigate the phase diagram using the Landau energy functional and derive coefficients of this energy functional within our mean-field theory. Second, we study the phase transition by solving the linearized gap equations. For both electronic and atomic systems, we find simultaneous existence of superconductivity and anti-ferromagnetism.

The paper is organized as follows. In section 2 and 3, we review the boson mediated attractive interactions for Bose–Fermi mixtures and electronic models, respectively. We devote section 4 to discuss our effective mean-field theory for the derivation of thermodynamic potential. In section 5, we introduced the Landau energy functional and then in section 6, we derive the gap equation and discuss our linearization scheme. In section 7, we discuss the generic two order parameter phase diagram within the Landau energy functional and derive Landau energy functional coefficients for both electronic and atomic models. In section 8, we discuss the critical temperatures and phase transitions using our linearized gap equations. Finally in section 9, we summarize the results and provide a general discussion.

2. Elementary excitation induced attractive interaction between fermions in Bose–Fermi mixture

In this section, we briefly review the effective interaction between fermions originated from the bosonic density fluctuations. When the lattice potential is strong, the atomic system in the two-dimensional (2D) square lattice can be modeled by the single band Hubbard model [63],

$$H_{bf} = -t_b \sum_{\langle i,j \rangle}\left(b_i^\dagger b_j + h.c\right) - t_f \sum_{\langle i,j \rangle,\sigma}\left(c_{i,\sigma}^\dagger c_{j,\sigma} + h.c\right) + \frac{U_{bb}}{2}\sum_i n_i^b(n_i^b - 1) + U_{bf}\sum_i n_i^b n_i^f + U_{ff}\sum_i n_{i,\uparrow} n_{j,\downarrow}, \quad (1)$$

where t_α is the boson ($\alpha = b$) and fermions ($\alpha = f$) tunneling amplitudes between neighboring sites i and j, respectively. The on-site boson–boson, boson–fermion, and fermion–fermion interactions are denoted by U_{bb}, U_{bf}, and U_{ff}, respectively. The operators $b_i(b_i^\dagger)$ are the on-site bosonic annihilation (creation) operators, and $c_{i,\sigma}$ are the on-site fermionic annihilation operators for pseudo spin $\sigma = \uparrow, \downarrow$. The Bosonic occupation number operator is $n_i^b = b_i^\dagger b_i$ and the fermionic occupation number operator for